Methane hydrate dissociation in presence of kinetic hydrate inhibitor through experiments and molecular dynamics simulation

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This work investigates the effect of kinetic hydrate inhibitor (KHIs) on methane hydrate dissociation. We have used a water soluble polymer as KHI and have studied its effect on the rate of decomposition of methane hydrate slurry and compared it with the decomposition rate in presence of polyvinylpyrrolidone (PVP). Effect of hydrate inhibitor on hydrate decomposition kinetics was studied at three different temperatures of 10, 15 and 20^{o}C. Experimental studies suggest that hydrate decomposition rate of methane hydrate in presence of KHIs is a function of temperature. Understanding the role of KHI in hydrate decomposition through molecular level simulations can bridge the gap between experiment and theory. Thus we have carried out a micro canonical ensemble molecular dynamics simulation of solid liquid interface of hydrate under certain concentration of PVP in amorphous water. Force field parameters for PVP are obtained and optimized against experimental density and heat of vaporization of PVP polymer.